# Semi–Analytic Approach to Higher–Order Corrections in Simple Muonic Bound Systems: Vacuum Polarization, Self–Energy and Radiative–Recoil

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**Abstract.** The current discrepancy of theory and experiment observed recently in muonic hydrogen necessitates a reinvestigation of all corrections to contribute to the Lamb shift in muonic hydrogen ($\mu$H), muonic deuterium ($\mu$D), the muonic $^3$He ion (denoted here as $\mu\,^3$He$^+$), as well as in the muonic $^4$He ion ($\mu\,^4$He$^+$). Here, we choose a semi-analytic approach and evaluate a number of higher-order corrections to vacuum polarization (VP) semi-analytically, while remaining integrals over the spectral density of VP are performed numerically. We obtain semi-analytic results for the second-order correction, and for the relativistic correction to VP. The self-energy correction to VP is calculated, including the perturbations of the Bethe logarithms by vacuum polarization. Subleading logarithmic terms in the radiative-recoil correction to the $2S$–$2P$ Lamb shift of order $\alpha(Z\alpha)^5\,\mu^3\,\ln(Z\alpha)/(m_\mu\,m_N)$ are also obtained. All calculations are nonperturbative in the mass ratio of orbiting particle and nucleus.
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## 1 Introduction

In simple muonic bound systems such as muonic hydrogen and deuterium ($\mu$H and $\mu$D) and muonic helium ions ($\mu\,^3$He$^+$ and $\mu\,^4$He$^+$), the mass ratio of the orbiting particle to the mass of the nucleus is larger than the fine-structure constant $\alpha$. The dominant radiative correction in these systems is given by electronic vacuum polarization, which screens the proton charge on a distance scale of the order of the electron Compton wavelength. Here, by "electronic" vacuum polarization, we refer to the modification of the photon propagator due to the creation and annihilation of electron-positron pairs. Due to the dominance of the vacuum-polarization energy shift (modification of the Coulomb force law at small distances), the $2S$ level is energetically lower in muonic systems as compared to the $2P_{1/2}$, reversing the ordering found in the hydrogen atom.

A characteristic property of simple bound muonic systems is the mass ratio

$$\xi_N = \frac{m_\mu}{m_N} \tag{1}$$

of orbiting particle and nucleus, which reads as

$$\xi_p = \frac{m_\mu}{m_p} = 0.112609\ldots \approx \tfrac{1}{9}\,, \tag{2a}$$

$$\xi_d = \frac{m_\mu}{m_d} = 0.0563327\ldots \approx \tfrac{1}{18} \tag{2b}$$

for muonic hydrogen and deuterium, and

$$\xi_{\mathrm{He}^3} = \frac{m_\mu}{m_{\mathrm{He}^3}} = 0.0376223\ldots \approx \tfrac{1}{26}\,, \tag{2c}$$

$$\xi_{\mathrm{He}^4} = \frac{m_\mu}{m_{\mathrm{He}^4}} = 0.0283465\ldots \approx \tfrac{1}{35} \tag{2d}$$

for muonic helium ions, where the latest recommended values of the masses have been used [1]. We here denote the masses of the helion nucleus and of the alpha particle as $m_{\mathrm{He}^3}$ and $m_{\mathrm{He}^4}$, respectively, in contrast to the muonic ions themselves, which we denote as $^3$He$^+$ and $^4$He$^+$.

For heavy muonic ions and atoms, the atomic binding-strength parameter is $Z\alpha$, where $Z$ is the nuclear charge number and the mass ratio $\xi_N$ of muon and atomic nucleus fulfills the inequality

$$\xi_N = \frac{m_\mu}{m_N} \ll Z\alpha < 1\,. \tag{3}$$

In heavy muonic ions, the external-field approximation (Dirac-Coulomb equation) gives an excellent result. The Dirac formalism takes relativistic effects (parameterized by $Z\alpha$) into account to all orders. For a system like positronium ($e^+e^-$) or true muonium ($\mu^+\mu^-$, Refs. [2–4]), the situation is opposite,

$$\alpha = Z\alpha \ll \xi_{\mu^+\mu^-} = \tfrac{1}{2} = \mathcal{O}(1)\,; \tag{4}$$

each muon is the "nucleus for the other one." In these systems, the Breit Hamiltonian is adequate [5]. The (static)

Breit Hamiltonian is exact in the muon-nucleus mass ratio but perturbative in $Z\alpha$. For muonic hydrogen, deuterium and muonic helium ions, the mass ratio $\xi_N$ is larger than the atomic binding strength parameter $Z\alpha$. These systems therefore "lean" more toward the situation encountered in positronium and true muonium than toward heavy muonic ions. It is thus preferable to treat the reduced-mass dependence of the corrections exactly (wherever possible). For completeness, we would like to stress here that $\mu$H is the only muonic atom studied so far (Ref. [6]) where the mass ratio is larger than the atomic binding strength parameter. In all other heavy muonic ions studied primarily in the 1970s and 1980s (for theoretical overviews see Refs. [7,8]), the binding parameter $Z\alpha$ is much larger than the mass ratio.

We proceed as follows. In Sec. 2, we evaluate second-order as well as relativistic corrections to vacuum polarization using our semi-analytic approach. The latter have been the subject of a recent paper [9]. In Sec. 3, the muon self-energy corrections to vacuum polarization are evaluated, taking into account the shift of the Bethe logarithms due to vacuum polarization. Finally, radiative-recoil corrections are treated in Sec. 4, and subleading single logarithmic terms are calculated, supplementing recent work [10]. Three appendices A—C complement the paper. We use natural units with $\hbar = c = \epsilon_0 = 1$.

## 2 Higher–Order Corrections to VP

### 2.1 Second–Order Correction to VP

For the calculation of VP effects in muonic systems, it is convenient to define the "massive" Coulomb potential

$$v_{\mathrm{vp}}(\lambda; r) = -\frac{Z\alpha}{r}\, \mathrm{e}^{-\lambda r}, \quad \lambda \equiv \lambda(\rho) = m_e\,\rho, \quad (5)$$

where $m_e$ is the electron mass and $\rho$ is a dimensionless spectral parameter for the vacuum polarization. It is also useful to define the linear operator $K$,

$$K[f(\rho)] = \frac{2\alpha}{3\pi} \int\limits_{2}^{\infty} \mathrm{d}\rho\, \frac{2+\rho^2}{\rho^3} \sqrt{1 - \frac{4}{\rho^2}}\, f(\rho)\,. \quad (6)$$

The reduced mass of the system is written as

$$\mu = \frac{m_\mu\, m_N}{m_\mu + m_N}\,, \qquad \beta_N = \frac{m_e}{Z\alpha\,\mu}\,. \quad (7)$$

The ratio of the muonic Bohr radius to the electron Compton wavelength is given by the ratios [11]

$$\beta_p = 0.7373836\ldots, \quad (8a)$$

$$\beta_d = 0.7000861\ldots, \quad (8b)$$

$$\beta_{\mathrm{He}^3} = 0.3438429\ldots, \quad (8c)$$

$$\beta_{\mathrm{He}^4} = 0.3407691\ldots \quad (8d)$$

Using formulas for the reduced Green function from Appendix B, and for analytic integrals from Appendix C, it is possible to analytically evaluate the following matrix element, which describes the second-order perturbation due to VP. For the $2P_{1/2}$–$2S_{1/2}$ Lamb shift difference

$$L^{(2)}(\rho_1, \rho_2) = \left\langle 2P \left| v_{\mathrm{vp}}(\lambda_1; r)\, \frac{1}{(E-H)'}\, v_{\mathrm{vp}}(\lambda_2; r) \right| 2P \right\rangle$$

$$- \left\langle 2S \left| v_{\mathrm{vp}}(\lambda_1; r)\, \frac{1}{(E-H)'}\, v_{\mathrm{vp}}(\lambda_2; r) \right| 2S \right\rangle\,, \quad (9)$$

where the prime denotes the reduced Green function, we find

$$L^{(2)}(\rho_1, \rho_2) = (Z\alpha)^2 \mu \left( \frac{[1+\beta_N(\rho_1+\rho_2)]^{-5}\, \mathcal{Q}}{12(1+\beta_N\rho_1)^5(1+\beta_N\rho_2)^5} + \frac{\beta_N^2\, [\rho_1^2 + \rho_2^2 + (\beta_N\rho_1\rho_2)^2]}{(1+\beta_N\rho_1)^4(1+\beta_N\rho_2)^4} \ln\left( \frac{(1+\beta_N\rho_1)(1+\beta_N\rho_2)}{1+\beta_N(\rho_1+\rho_2)} \right) \right)\,. \quad (10)$$

Here, $\mathcal{Q} \equiv \mathcal{Q}(\beta_N; \rho_1, \rho_2)$ is a polynomial in the three arguments, symmetric in $\rho_1$ and $\rho_2$ and rather compact,

$$\mathcal{Q} = -3\rho_1^2 + 18\beta_N^2\rho_1^4 + 24\beta_N^3\rho_1^5 + 9\beta_N^4\rho_1^6 - 24\beta_N\rho_1^2\rho_2 - 3\beta_N^2\rho_1^3\rho_2 + 99\beta_N^3\rho_1^4\rho_2 + 111\beta_N^4\rho_1^5\rho_2 + 33\beta_N^5\rho_1^6\rho_2$$

$$- 75\beta_N^2\rho_1^2\rho_2^2 - 189\beta_N^3\rho_1^3\rho_2^2 - 33\beta_N^4\rho_1^4\rho_2^2 + 39\beta_N^5\rho_1^5\rho_2^2 + 12\beta_N^6\rho_1^6\rho_2^2 - 142\beta_N^4\rho_1^3\rho_2^3 - 62\beta_N^5\rho_1^4\rho_2^3$$

$$+ 84\beta_N^6\rho_1^5\rho_2^3 + 36\beta_N^7\rho_1^6\rho_2^3 + 74\beta_N^6\rho_1^4\rho_2^4 + 120\beta_N^7\rho_1^5\rho_2^4 + 12\beta_N^8\rho_1^6\rho_2^4 - 12\beta_N^8\rho_1^5\rho_2^5 + (\rho_1 \leftrightarrow \rho_2)\,. \quad (11)$$

The energy shift is given as

$$\Delta E^{(2)} = K_1 \left[ K_2 \left[ L^{(2)}(\rho_1, \rho_2) \right] \right]\,, \quad (12)$$

where $K_1$ and $K_2$ are the generalizations of the operator in Eqs. (6) to integration variables $\rho_1$ and $\rho_2$. Our semi-analytic approach allows us to evaluate the remain-
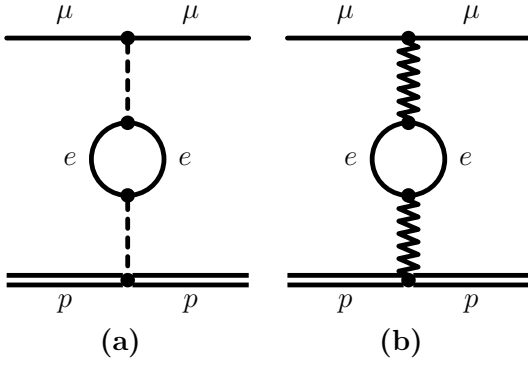
**Fig. 1.** Feynman diagrams for the relativistic correction to vacuum polarization in the two-body system of a muon and a nucleus. The electron-positron pair in the loop is denoted by the symbol $e$. Diagram (a) is the Coulomb photon exchange, given by the 00-component of the "massive" photon propagator, whereas diagram (b) is the magnetic exchange, corresponding to the spatial components of the "massive" photon propagator.
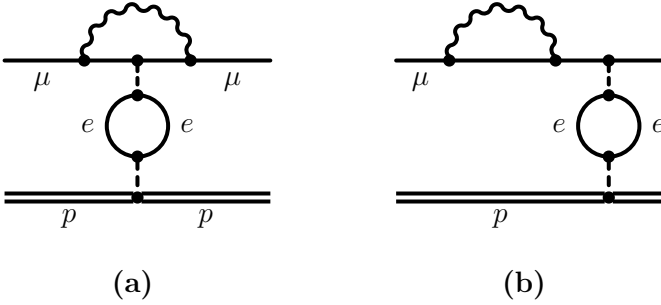


**Fig. 2.** Feynman diagrams for the self-energy correction to vacuum polarization in a simple muonic bound system. Diagram (a) represents the vacuum-polarization insertion into the exchanged photon in the vertex correction, whereas diagram (b) represents the wave function correction to the self energy due to vacuum polarization.

ing two-dimensional numerical integrals to essentially arbitrary accuracy.

For the muonic systems of interest, the second-order shift is found as

$$\Delta E^{(2)}(\mu\mathrm{H}) = 0.150897\,\mathrm{meV}\,, \tag{13a}$$

$$\Delta E^{(2)}(\mu\mathrm{D}) = 0.172023\,\mathrm{meV}\,, \tag{13b}$$

$$\Delta E^{(2)}(\mu\,{}^3\mathrm{He}^+) = 1.677290\,\mathrm{meV}\,, \tag{13c}$$

$$\Delta E^{(2)}(\mu\,{}^4\mathrm{He}^+) = 1.707588\,\mathrm{meV}\,. \tag{13d}$$

For muonic hydrogen, we confirm the entry in Eq. (28) of Ref. [11], and for $\mu\,{}^4\mathrm{He}^+$, we confirm the results given

in Eq. (38) and (39) of Ref. [12]. Our semi-analytic approach eliminates any conceivable numerical inaccuracy as the reason for (part of) the experimental-theoretical disagreement [6].

## 2.2 Relativistic Correction to VP

The relativistic correction $\delta w = \sum_{i=1}^{4} \delta w_i$ to the Breit interaction, relevant for the $2P_{1/2}$–$2S_{1/2}$ Lamb shift, is given as the sum of four terms [10, 11]

$$\delta w_1 = \frac{Z\alpha}{8} \left( \frac{1}{m_\mu^2} + \frac{\delta_I}{m_N^2} \right) \left( 4\pi\delta^3(r) - \frac{\lambda^2}{r}\,\mathrm{e}^{-\lambda r} \right)\,, \tag{14}$$

$$\delta w_2 = -\frac{Z\alpha\lambda^2\mathrm{e}^{-\lambda r}}{4m_\mu m_N r} \left( 1 - \frac{\lambda r}{2} \right)\,,$$

$$\delta w_3 = -\frac{Z\alpha\,\mathrm{e}^{-\lambda r}}{4m_\mu m_N}\, p^i \left( \frac{\delta^{ij}}{r} + \frac{1+\lambda r}{r^3}\,r^i r^j \right)\, p^j\,,$$

$$\delta w_4 = Z\alpha \left( \frac{1}{4m_\mu^2} + \frac{1}{2m_\mu m_N} \right) \frac{\mathrm{e}^{-\lambda r}\,(1+\lambda r)}{r^3}\,\boldsymbol{\sigma}\cdot\boldsymbol{L}\,,$$

where $\delta_I$ is one for half-integer nuclear spin and zero for integer nuclear spin. For the relevant Feynman diagrams, see Fig. 1. The massive Breit Hamiltonian (2.2) is a generalization of the ordinary Breit Hamiltonian briefly revisited in Appendix A. The relativistic correction to VP is the sum of first-order and second-order perturbations,

$$\delta E_{\mathrm{vp}} = \delta E^{(1)} + \delta E^{(2)}\,, \tag{15a}$$

$$\delta M^{(1)} = \langle n\ell_j |\,\delta w\,| n\ell_j \rangle\,, \tag{15b}$$

$$\delta M^{(2)} = 2 \left\langle n\ell_j \left| \delta H \left( \frac{1}{E_{n\ell} - H} \right)' v_{\mathrm{vp}} \right| n\ell_j \right\rangle\,, \tag{15c}$$

$$\delta E^{(1)} = K[\delta M^{(1)}]\,, \qquad \delta E^{(2)} = K[\delta M^{(2)}]\,, \tag{15d}$$

$$\delta E_{\mathrm{vp}} = \delta E^{(1)} + \delta E^{(2)}\,. \tag{15e}$$

Here, the reference state has principal quantum number $n$, orbital angular momentum $\ell$, and total angular momentum $j$. For the second-order matrix elements $\delta M^{(2)}$, one needs the explicit formulas for the reduced Green function given in Appendix B. The radial integrals can be performed analytically using formulas given in Appendix C. Finally, the matrix elements $\delta M^{(1)}$ and $\delta M^{(2)}$ can be evaluated analytically.

We present explicit results for the matrix elements $\delta M^{(1)}$ and $\delta M^{(2)}$ [see Eqs. (15b) and (15c)], assuming $\delta_I = 1$, for the muonic bound systems under investigation, in terms of the parameters $Z\alpha$, $\xi_N$ [defined in Eq. (1)], and $\beta_N$ [defined in Eq. (7)],

$$\delta M^{(1)}(2P_{\frac{1}{2}}) = -\frac{(Z\alpha)^4\,\mu\,\left[2 + 10\,\xi_N + 4\beta_N\rho(2 + 7\xi_N) + 3(\beta_N\,\rho)^2(3 + 6\xi_N + \xi_N^2)\right]}{96\,(1 + \xi_N)^2\,(1 + \beta_N\,\rho)^4}\,, \tag{16a}$$

$$\delta M^{(1)}(2S_{\frac{1}{2}}) = \frac{(Z\alpha)^4\,\mu\,\left\{2\left[1 + \xi_N^2 - \xi_N\,(1 + \beta_N\,\rho)^2\,(3 + 4\beta_N\rho)\right] + \beta_N\rho\,(1 + \xi_N^2)\,[8 + \beta_N\,\rho(11 + 8\beta_N\rho)]\right\}}{32\,(1 + \xi_N)^2\,(1 + \beta_N\,\rho)^4}\,, \tag{16b}$$

$$\delta M^{(2)}(2P_{\frac{1}{2}}) = \frac{(Z\alpha)^4\,\mu\,\left[f(\beta_N,\rho,\xi_N) - 8(\beta_N\rho)^2\,(2 + \xi_N + \xi_N^2) - 8\,(1 + \beta_N\,\rho)\,(3 + 6\xi_N + 2\xi_N^2)\,\ln(1 + \beta_N\,\rho)\right]}{96\,(1 + \xi_N)^2\,(1 + \beta_N\,\rho)^5}\,, \tag{16c}$$

$$f(\beta_N,\rho,\xi_N) = -13 - 23\,\xi_N - 7\,\xi_N^2 - \beta_N\,\rho\,\left(41 + 67\,\xi_N + 19\,\xi_N^2\right)\,, \tag{16d}$$

$$\delta M^{(2)}(2S_{\frac{1}{2}}) = \frac{(Z\alpha)^4\,\mu\,\left[g(\beta_N,\rho,\xi_N) - 8\,(\beta_N\,\rho)^4\,(\xi_N - 1)^2 - 8\,(1 + \xi_N)^2\,(1 + \beta_N\,\rho)\,\left(1 + 2(\beta_N\,\rho)^2\right)\,\ln(1 + \beta_N\,\rho)\right]}{32\,(1 + \xi_N)^2\,(1 + \beta_N\,\rho)^5}\,, \tag{16e}$$

$$g(\beta_N,\rho,\xi_N) = -7 - 5\xi_N - 7\xi_N^2 - 9\beta_N\rho\,(3 + \xi_N + 3\xi_N) - 2(\beta_N\rho)^2(15 - 13\xi_N + 15\xi_N^2) - 10(\beta_N\rho)^3(3 - \xi_N + 3\xi_N^2). \tag{16f}$$

This reduces the calculation of $\delta E^{(1)}$ and $\delta E^{(2)}$ to simple numerical integrals over the spectral representation of the vacuum polarization ($K$ operator). We have not attempted here to carry out the remaining integrals over $\rho$ analytically because the integral representation allows us to evaluate the relativistic correction to VP to essentially arbitrary accuracy.

For the $2P_{1/2}$–$2S_{1/2}$ Lamb shift, we indicate the difference as $\Delta E_{\mathrm{vp}} = \delta E_{\mathrm{vp}}(2P_{1/2}) - \delta E_{\mathrm{vp}}(2S_{1/2})$,

$$\Delta E_{\mathrm{vp}}(\mu\mathrm{H}) = 0.018759\,\mathrm{meV}\,, \tag{17a}$$

$$\Delta E_{\mathrm{vp}}(\mu\mathrm{D}) = 0.021781\,\mathrm{meV}\,, \tag{17b}$$

$$\Delta E_{\mathrm{vp}}(\mu\,^3\mathrm{He}^+) = 0.509344\,\mathrm{meV}\,, \tag{17c}$$

$$\Delta E_{\mathrm{vp}}(\mu\,^4\mathrm{He}^+) = 0.521104\,\mathrm{meV}\,. \tag{17d}$$

The relativistic correction to vacuum polarization is represented by the tree-level Feynman diagrams in Fig. 1, which represent vacuum-polarization insertions in the Coulomb and magnetic exchange, with relativistic wave functions in the in and out states. Our results are in agreement with those recently reported in Ref. [10]. This concludes our semi-analytic rederivation of the relativistic corrections to vacuum polarization, with proper account of the reduced-mass dependence.

## 3 Self–Energy Correction to VP

In Sec. 3.2 of Ref. [13], the self-energy correction to vacuum polarization has been discussed. In the cited reference, a partially nonperturbative approach has been chosen in order to evaluate certain matrix elements in a nonperturbative framework, using exact wave functions

for the Schrödinger-Coulomb problem, evaluated on exact operators that take vacuum polarization into account. Here, we compare the nonperturbative to a perturbative treatment of the vacuum-polarization potential $V_{\mathrm{vp}}$. The Uehling potential is added to the Schrödinger Hamiltonian by the replacement $V \to V + V_{\mathrm{vp}}$. The effect of high-energy virtual photons in the self-energy loops given in Fig. 2 can thus be expressed in terms of the Dirac $F_1$ form factor acting on the vacuum polarization potential $V_{\mathrm{vp}}$. When rewritten in terms of the noncovariant photon energy cutoff $\epsilon$, which is a convenient overlapping parameter in Lamb shift calculations [14], we have in first order in $V_{\mathrm{vp}}$,

$$\delta E_H = \frac{\alpha}{3\pi m_\mu^2}\left[\ln\left(\frac{m_\mu}{2\epsilon}\right) + \frac{10}{9}\right]\left(\langle n\ell_j\,|\,\boldsymbol{\nabla}^2 V_{\mathrm{vp}}\,|\,n\ell_j\rangle\right.$$
$$\left. + 2\left\langle n\ell_j\,\middle|\,V_{\mathrm{vp}}\left(\frac{1}{E - H}\right)'\boldsymbol{\nabla}^2 V\,\middle|\,n\ell_j\right\rangle\right)\,. \tag{18}$$

This is equivalent to expanding Eq. (3.7) of Ref. [13] to first order in the vacuum–polarization potential. The correction $\delta E_H$ to the high-energy part is expressed in terms of a parameter $V_{61}$,

$$\delta E_H = \frac{\alpha^2\,(Z\alpha)^4\,\mu^3}{\pi^2 m_\mu^2\,n^3}\,V_{61}\left\{\ln\left(\frac{m_\mu}{2\epsilon}\right) + \frac{10}{9}\right\}\,. \tag{19}$$

We find, using techniques similar to those employed in Sec. 2,

$$V_{61}(2P_{1/2}; \mu\text{H}) = -0.02327\,, \qquad (20\text{a})$$

$$V_{61}(2P_{1/2}; \mu\text{D}) = -0.02453\,, \qquad (20\text{b})$$

$$V_{61}(2P_{1/2}; \mu\,^3\text{He}^+) = -0.04345\,, \qquad (20\text{c})$$

$$V_{61}(2P_{1/2}; \mu\,^4\text{He}^+) = -0.04369\,. \qquad (20\text{d})$$

For the $2S_{1/2}$ state, the results are

$$V_{61}(2S_{1/2}; \mu\text{H}) = 3.08601\,, \qquad (21\text{a})$$

$$V_{61}(2S_{1/2}; \mu\text{D}) = 3.18785\,, \qquad (21\text{b})$$

$$V_{61}(2S_{1/2}; \mu\,^3\text{He}^+) = 4.71872\,, \qquad (21\text{c})$$

$$V_{61}(2S_{1/2}; \mu\,^4\text{He}^+) = 4.73968\,. \qquad (21\text{d})$$

The results for $\mu$H confirm the entries in Eq. (3.8) of Ref. [13], where a nonperturbative approach in the vacuum-polarization potential was employed. The correction due to the anomalous magnetic moment of the electron reads as

$$\delta E_M = \frac{\alpha}{4\pi m_\mu^2} \left( \left\langle n\ell_j \left| \frac{1}{r} \frac{\partial V_{\text{vp}}}{\partial r} (\boldsymbol{\sigma}\cdot\boldsymbol{L}) \right| n\ell_j \right\rangle \right.$$

$$\left. + 2 \left\langle n\ell_j \left| V_{\text{vp}} \left( \frac{1}{E-H} \right)' \frac{1}{r} \frac{\partial V}{\partial r} (\boldsymbol{\sigma}\cdot\boldsymbol{L}) \right| n\ell_j \right\rangle \right)$$

$$= \frac{\alpha^2 (Z\alpha)^4 \mu^3}{\pi^2 m_\mu^2 n^3} M_{60}\,. \qquad (22)$$

The matrix element $M_{60}$ is nonvanishing for $P$ states,

$$M_{60}(2P_{1/2}; \mu\text{H}) = -0.04276\,, \qquad (23\text{a})$$

$$M_{60}(2P_{1/2}; \mu\text{D}) = -0.04656\,, \qquad (23\text{b})$$

$$M_{60}(2P_{1/2}; \mu\,^3\text{He}^+) = -0.13396\,, \qquad (23\text{c})$$

$$M_{60}(2P_{1/2}; \mu\,^4\text{He}^+) = -0.13556\,. \qquad (23\text{d})$$

For $S$ states, we have $M_{60}(2S_{1/2}) = 0$ in view of angular symmetry. For the $2P$ state, we here take the opportunity to correct the result given in Eq. (3.10) of Ref. [13]. The correction has negligible influence on the numerical result reported below in Eq. (29) for muonic hydrogen.

The low-energy part is conveniently expressed as

$$\delta E_L = \frac{\alpha^2 (Z\alpha)^4 \mu^3}{\pi^2 m_\mu^2 n^3} \left[ V_{61} \ln\left( \frac{\epsilon}{(Z\alpha)^2\mu} \right) - \frac{4}{3} L_{60} \right]\,, \qquad (24)$$

where the $V_{61}$ term leads to a cancellation of the $\epsilon$ parameter. The coefficient $L_{60}$ gives the modification of the Bethe logarithm due to the Uehling potential. Numerically, we find for $2P_{1/2}$,

$$L_{60}(2P_{1/2}; \mu\text{H}) = -0.014559\,, \qquad (25\text{a})$$

$$L_{60}(2P_{1/2}; \mu\text{D}) = -0.015446\,, \qquad (25\text{b})$$

$$L_{60}(2P_{1/2}; \mu\,^3\text{He}^+) = -0.032293\,, \qquad (25\text{c})$$

$$L_{60}(2P_{1/2}; \mu\,^4\text{He}^+) = -0.032573\,, \qquad (25\text{d})$$

whereas for $2S_{1/2}$,

$$L_{60}(2S_{1/2}; \mu\text{H}) = 11.176\,, \qquad (26\text{a})$$

$$L_{60}(2S_{1/2}; \mu\text{D}) = 11.464\,, \qquad (26\text{b})$$

$$L_{60}(2S_{1/2}; \mu\,^3\text{He}^+) = 15.640\,, \qquad (26\text{c})$$

$$L_{60}(2S_{1/2}; \mu\,^4\text{He}^+) = 15.696\,. \qquad (26\text{d})$$

The total self-energy vacuum-polarization correction to the $2P$–$2S$ Lamb shift then is

$$\delta E_{\text{svp}} = \delta E_H + \delta E_M + \delta E_L = \frac{\alpha^2 (Z\alpha)^4 \mu^3}{\pi^2 m_\mu^2 n^3} \qquad (27)$$

$$\times \left\{ \left[ \ln\left( \frac{m_\mu}{2(Z\alpha)^2\mu} \right) + \frac{10}{9} \right] \Delta V_{61} + \Delta M_{60} - \frac{4}{3}\Delta L_{60} \right\}\,,$$

where

$$\Delta V_{61} = V_{61}(2P_{1/2}) - V_{61}(2S_{1/2})\,, \qquad (28\text{a})$$

$$\Delta M_{60} = M_{60}(2P_{1/2}) - M_{60}(2S_{1/2})\,, \qquad (28\text{b})$$

$$\Delta L_{60} = L_{60}(2P_{1/2}) - L_{60}(2S_{1/2})\,. \qquad (28\text{c})$$

The final numerical values for the contributions to the $2P_{1/2}$–$2S_{1/2}$ Lamb shift are given as

$$\Delta E_{\text{svp}}(\mu\text{H}) = -0.00254\,\text{meV}\,, \qquad (29\text{a})$$

$$\Delta E_{\text{svp}}(\mu\text{D}) = -0.00306\,\text{meV}\,, \qquad (29\text{b})$$

$$\Delta E_{\text{svp}}(\mu\,^3\text{He}^+) = -0.06269\,\text{meV}\,, \qquad (29\text{c})$$

$$\Delta E_{\text{svp}}(\mu\,^4\text{He}^+) = -0.06462\,\text{meV}\,. \qquad (29\text{d})$$

## 4 Recoil Correction to VP

### 4.1 Formulation of Radiative Recoil

The first genuine two-body energy correction beyond the frequency-independent part of the Breit interaction involves a photon-frequency dependent transverse exchange and a relativistic two-photon exchange [15]. For the $1S$
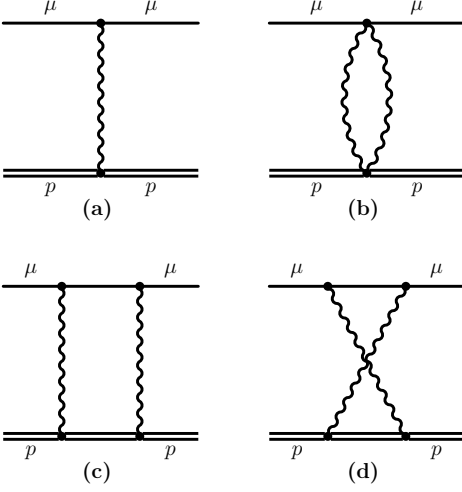
**Fig. 3.** Typical Feynman diagrams for the recoil correction. Diagram (a) is the frequency-dependent part of the Breit interaction, (b) is the seagull exchange graph, and (c) and (d) are two-photon exchange graphs.

state, the corresponding energy shift was calculated in Ref. [16], which is why the recoil correction is commonly referred to as the Salpeter correction, and the result was generalized to an arbitrary excited state in Ref. [17]. The correction reads, for an individual state with principal quantum number $n$ and angular momentum $\ell$,

$$
E_R = \frac{(Z\alpha)^5 \mu^3}{\pi m_\mu m_N n^3} \left\{ \frac{2}{3} \delta_{\ell 0} \ln\left(\frac{1}{Z\alpha}\right) - \frac{8}{3} \ln k_0 - \frac{\delta_{\ell 0}}{9} \right.
$$

$$
\left. - \frac{7a_n}{3} - \frac{2\delta_{\ell 0}}{m_\mu^2 - m_N^2} \left[ m_\mu^2 \ln\left(\frac{m_N}{\mu}\right) - m_N^2 \ln\left(\frac{m_\mu}{\mu}\right) \right] \right\} ,
\tag{30}
$$

where

$$
a_n = -2 \left[ \ln\left(\frac{2}{n}\right) + 1 + \frac{1}{2n} + \Psi(n) + \gamma_E \right] ,
\tag{31}
$$

and $\Psi(n) = \sum_{k=1}^{n-1} k^{-1}$ denotes the logarithmic derivative of the Gamma function.

For reference, we evaluate the recoil correction for the $2P_{1/2}$–$2S_{1/2}$ Lamb shift, for the muonic systems under investigation,

$$
\Delta E_R(\mu\mathrm{H}) = -0.044971\,\mathrm{meV} ,
\tag{32a}
$$

$$
\Delta E_R(\mu\mathrm{D}) = -0.026561\,\mathrm{meV} ,
\tag{32b}
$$

$$
\Delta E_R(\mu\,{}^3\mathrm{He}^+) = -0.558107\,\mathrm{meV} ,
\tag{32c}
$$

$$
\Delta E_R(\mu\,{}^4\mathrm{He}^+) = -0.433032\,\mathrm{meV} .
\tag{32d}
$$

We thus confirm the result indicated in Eq. (66) of Ref. [12] and the results given in Tables 3–6 of Ref. [18].

According to the derivation presented in Ref. [15], the recoil correction is formulated in terms of four corrections.
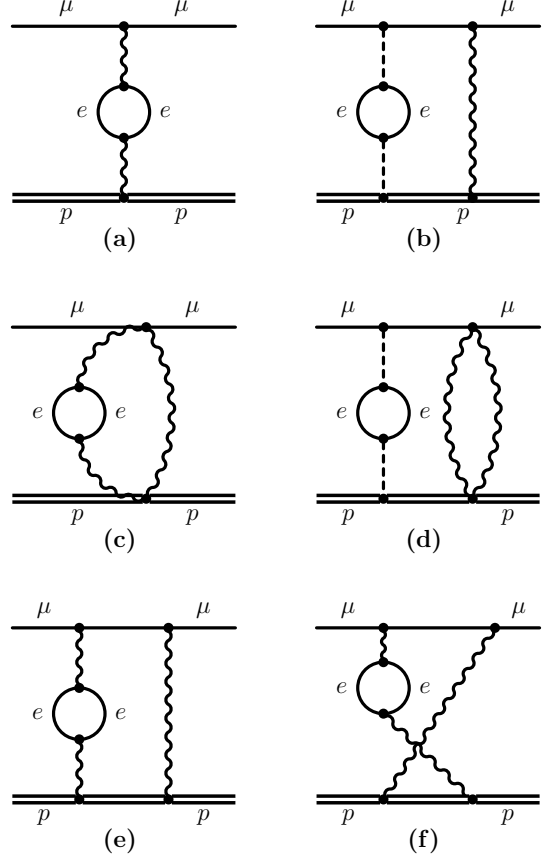


**Fig. 4.** The six Feynman diagrams for the vacuum-polarization correction to recoil (radiative-recoil correction) of relative order $\alpha$, in muonic and antiprotonic systems. The electron-positron pair in the loop is denoted by the symbol $e$. Coulomb photons are denoted by dashed lines.

Two of these are associated with the photon-frequency dependent part of the Breit interaction [see Fig. 3(a)]. The other two are associated with two-photon exchange [see Fig. 3(b), (c) and (d)]. The frequency-dependent one-photon exchange in Fig. 3(a) leads to a low-energy part $E_L$ where the photon frequency fulfills $\omega \ll Z\alpha\mu$ and therefore is small against the orbiting particle momentum, and a middle-energy part $E_M$, where $\omega \gg Z\alpha\mu$. The two parts are separated by an overlapping parameter. The frequency-dependent part of the Breit interaction is described by $E_L$ and $E_M$.

For low photon frequencies, the two-photon exchange is described by the seagull graph in Fig. 3(b). The seagull exchange energy correction $E_S$ effectively represents the "low-energy part" of the two-photon exchange, whereas the high-energy part $E_H$ describes a local operator, with both virtual photon momenta and the momenta of the constituent particles being large [see Figs. 3(c) and (d)]. It contributes only for $S$ states. A second overlapping parameter cancels between $E_S$ and $E_H$. The seagull exchange diagram in Fig. 3(b) exists in nonrelativistic QED (NRQED) as opposed to fully relativistic QED, where two-photon emission out of the same vertex is forbidden. Indeed, the seagull diagram follows from the two-photon exchange di-

agram of relativistic QED (two-photon emission) in the limit of soft photons and negative-energy virtual fermion states (the fermion lines would have a "$Z$" shape in time-ordered perturbation theory).

The radiative-recoil correction of order $\alpha(Z\alpha)^5\mu^3/(m_\mu m_N)$ is the perturbation of the recoil correction of order $(Z\alpha)^5\mu^3/(m_\mu m_N)$ by an order-$\alpha$ vacuum polarization, and is calculated here for simple muonic bound systems. Because the correction is numerically small, we restrict our attention to the leading logarithms. The contributing diagrams at relative order $\alpha$ are given in Fig. 4. One might expect a seventh diagram to contribute, with a VP correction to a Coulomb photon exchange in the seagull graph, where the seagull vertices connect to the muon and proton/deuteron lines on opposite sides of the Coulomb/Uehling exchange. However, the seventh diagram only contributes at relative order $\alpha(Z\alpha)$ and is not considered here.

### 4.2 Logarithm from Middle– and Low–Energy Part

As evident from the derivation in Ref. [15], the logarithmic term in Eq. (30) can be broken down as follows,

$$E_R^{\log} = \frac{(Z\alpha)^5\mu^3}{\pi m_\mu m_N n^3}\left(\frac{8}{3}-2\right)\delta_{\ell 0}\ln\left(\frac{1}{Z\alpha}\right), \qquad (33)$$

where the term with the prefactor "8/3" comes from the sum of the middle- and low-energy parts. The first logarithmic term in the recoil correction (due to the middle- and low-energy parts) can thus be expressed as a matrix element of the Laplacian of the Coulomb potential $V$,

$$E_L = \frac{2Z\alpha}{3\pi\, m_\mu m_N}\left\langle n\ell_j\left|\boldsymbol{\nabla}^2 V\right|n\ell_j\right\rangle\ln\left(\frac{1}{Z\alpha}\right). \qquad (34)$$

Perturbing the matrix element by the vacuum-polarization potential, we obtain the following logarithmic ($L$) term in the radiative-recoil correction,

$$\begin{aligned}\delta E_L &= \frac{2Z\alpha\,\ln[(Z\alpha)^{-1}]}{3\pi\,m_\mu m_N}\left(\left\langle n\ell_j\left|\boldsymbol{\nabla}^2 V_{\rm vp}\right|n\ell_j\right\rangle\right.\\ &\left.+ 2\left\langle n\ell_j\left|\boldsymbol{\nabla}^2 V\left(\frac{1}{E_{nP}-H_0}\right)' V_{\rm vp}\right|n\ell_j\right\rangle\right)\\ &= \frac{\alpha}{\pi}\,\xi_N\,\frac{2(Z\alpha)^5\mu^3}{\pi\,m_\mu^2 n^3}V_{61}\ln\left(\frac{1}{Z\alpha}\right).\end{aligned} \qquad (35)$$

This result is spin-independent and in full agreement with Eq. (5.165) of a recent unpublished work (Ref. [19]), where for $P$ states, nonlogarithmic terms are calculated as well (we only consider the leading logarithms here). Results for $V_{61}$ can be found in Eq. (20a).

For the $2P_{1/2}$–$2S_{1/2}$ Lamb shift, indicated by the prefix $\Delta$, the correction evaluates to

$$\Delta E_L(\mu{\rm H}) = -0.000505\,{\rm meV}, \qquad (36a)$$

$$\Delta E_L(\mu{\rm D}) = -0.000295\,{\rm meV}, \qquad (36b)$$

$$\Delta E_L(\mu\,{}^3{\rm He}^+) = -0.005724\,{\rm meV}, \qquad (36c)$$

$$\Delta E_L(\mu\,{}^4{\rm He}^+) = -0.004431\,{\rm meV}. \qquad (36d)$$

This concludes the treatment of the logarithmic terms in the radiative-recoil correction due to the diagrams in Fig. 2(a) and (b). It is *not* the leading logarithmic term in the radiative-recoil correction.

### 4.3 Logarithm from Seagull and High–Energy Part

The mechanism for the generation of logarithmic terms in the seagull part is different from the middle- and low-energy parts and cannot be traced to a perturbative modification of the matrix element in the term (34). For the first logarithmic contribution, it is sufficient to consider the seagull exchange diagram given in Fig. 4(c); the high-energy terms from Fig. 4(e) and (f) cancel an intermediate overlapping parameter and their contribution is not needed in the evaluation of the logarithmic terms. The seagull term, with a vacuum polarization insertion in the exchanged photon, is given as

$$\delta E_S = -\frac{e^4}{2m_\mu m_N}\,K\left[\int\frac{{\rm d}^3 k_1}{(2\pi)^3}\frac{{\rm d}^3 k_2}{(2\pi)^3}\frac{1}{\omega_1\,k_2}\frac{1}{\omega_1 + k_2}\right. \qquad (37)$$

$$\left(\delta^{ij} - \frac{k_1^i\,k_1^j}{\omega_1^2}\right)\left(\delta^{ij} - \frac{k_2^i\,k_2^j}{k_2^2}\right)\left]\left\langle n\ell_j|{\rm e}^{{\rm i}\,(\boldsymbol{k}_1+\boldsymbol{k}_2)\cdot\boldsymbol{r}}|n\ell_j\right\rangle\right.$$

where $\omega_1 = \sqrt{\boldsymbol{k}_1^2 + \lambda^2} = \sqrt{\boldsymbol{k}_1^2 + (m_e\,\rho)^2}$ is the photon frequency for massive photons. From this integral, using a cutoff $\Lambda$ as in Eq. (27) of Ref. [15] as an overlapping parameter that separates the integration region from the high-energy part, we extract the following logarithmic correction terms, which contribute only for $S$ states,

$$\delta E_S = \frac{4\alpha\,(Z\alpha)^5\,\mu^3}{3\pi^2 m_\mu m_N n^3}\,\delta_{\ell 0} \qquad (38)$$

$$\times\left[-\ln^2\left(4Z\alpha\beta_N^2\right) + \ln(2\beta_N)\ln\left(4Z\alpha\beta_N^2\right)\right].$$

The double logarithmic term is formally leading (we here confirm the result of Ref. [10]). This correction evaluates to

$$\Delta E_S(\mu{\rm H}) = 0.000414\,{\rm meV}, \qquad (39a)$$

$$\Delta E_S(\mu{\rm D}) = 0.000251\,{\rm meV}, \qquad (39b)$$

$$\Delta E_S(\mu\,{}^3{\rm He}^+) = 0.006648\,{\rm meV}, \qquad (39c)$$

$$\Delta E_S(\mu\,{}^4{\rm He}^+) = 0.005174\,{\rm meV}. \qquad (39d)$$

There is a second correction for $S$ states. It is given by the wave function correction to the leading seagull logarithm

$$E_S = -\frac{2(Z\alpha)^2}{m_\mu\,m_p}\,|\phi_{n\ell}(0)|^2\,\ln\left(\frac{1}{Z\alpha}\right),\qquad(40)$$

where $\phi_{n\ell}$ is the nonrelativistic Schrödinger wave function. We note that this term cannot be traced to the expectation value of the Laplacian of the Coulomb potential, $\langle\boldsymbol{\nabla}^2 V\rangle$, and therefore the formalism leading to the result in Eq. (35) is not applicable. The wave function correction due to the potential $v_{\rm vp}$ is

$$\delta\phi_{nS} = \left(\frac{1}{E-H}\right)' v_{\rm vp}|\phi_{nS}\rangle.\qquad(41)$$

At the origin, the correction can be expressed as ($2S$ state)

$$\delta\phi_{2S}(0) = \frac{(Z\alpha\mu)^{5/2}}{4\sqrt{2\pi}(\lambda+Z\alpha\mu)^5}\left[4\lambda^4 + 12(Z\alpha\mu)\lambda^3\right.$$

$$+4(Z\alpha\mu)^2\lambda^2 + 11(Z\alpha\mu)^3\lambda + 3(\alpha\mu)^4\right]$$

$$+\frac{(Z\alpha\mu)^{7/2}\left(2\lambda^2+(\alpha\mu)^2\right)}{\sqrt{2\pi}(\lambda+Z\alpha\mu)^4}\ln\left(1+\frac{\lambda}{Z\alpha\,\mu}\right).\qquad(42)$$

The corresponding logarithmic energy correction for an $nS$ state due to the wave function correction reads as

$$\delta E_W = -\frac{2\,(Z\alpha)^2}{m_\mu m_N}\,K\,[\,2\phi_{n\ell}(0)\,\delta\phi_{n\ell}(0)\,]\ln\left(\frac{1}{Z\alpha}\right)\quad(43)$$

for an individual state. A numerical evaluation for the Lamb shift ($2P_{1/2}$–$2S_{1/2}$ energy difference) leads to the results (again denoted by the prefix $\Delta$ instead of $\delta$),

$$\Delta E_W(\mu\mathrm{H}) = 0.000228\,\mathrm{meV},\qquad(44\mathrm{a})$$

$$\Delta E_W(\mu\mathrm{D}) = 0.000138\,\mathrm{meV},\qquad(44\mathrm{b})$$

$$\Delta E_W(\mu\,^3\mathrm{He}^+) = 0.004017\,\mathrm{meV},\qquad(44\mathrm{c})$$

$$\Delta E_W(\mu\,^4\mathrm{He}^+) = 0.003123\,\mathrm{meV},\qquad(44\mathrm{d})$$

which is of the expected magnitude. The correction $\Delta E_W$ corresponds to the diagram in Fig. 4(d). The seagull and high-energy parts do not generate any logarithmic radiative-recoil corrections for $P$ states.

### 4.4 Total Logarithmic Radiative–Recoil Correction

For the Lamb shift, the total logarithmic radiative-recoil correction is given as the sum

$$\Delta E_{RR} = \Delta E_L + \Delta E_S + \Delta E_W.\qquad(45)$$

It evaluates to

$$\Delta E_{RR}(\mu\mathrm{H}) = 0.000136\,\mathrm{meV},\qquad(46\mathrm{a})$$

$$\Delta E_{RR}(\mu\mathrm{D}) = 0.000093\,\mathrm{meV},\qquad(46\mathrm{b})$$

$$\Delta E_{RR}(\mu\,^3\mathrm{He}^+) = 0.004941\,\mathrm{meV},\qquad(46\mathrm{c})$$

$$\Delta E_{RR}(\mu\,^4\mathrm{He}^+) = 0.003867\,\mathrm{meV}.\qquad(46\mathrm{d})$$

The results are numerically small and suppressed with respect to the leading recoil correction given in Eq. (32) by a factor $\alpha$.

There is some numerical cancellation between the leading squared logarithm given by the first term on the right-hand side of Eq. (38) and the subleading single logarithms.

## 5 Conclusions

The conclusions of this paper are twofold. The first conclusion is that a number of nontrivial higher-order corrections to the Lamb shift in simple muonic systems ($\mu$H, $\mu$D, $\mu\,^3$He$^+$, $\mu\,^4$He$^+$) can be evaluated semi-analytically. Certain well-defined, remaining one- or two-dimensional numerical integrals can easily be evaluated to essentially arbitrary accuracy. The second-order VP shift (Sec. 2.1) has been investigated numerically in a number of previous works [11–13], and we here confirm these results using our semi-analytic approach [see Eq. (9)] and complement the literature with a result for $\mu\,^3$He$^+$. The second-order correction is otherwise easy to evaluate numerically; the only advantage of our approach is that the integral representation easily allows us to evaluate the correction to essentially arbitrary accuracy, yielding an additional confirmation for the literature values. The relativistic correction to VP (with a proper account of the reduced-mass dependence) is analyzed in Sec. 2.2. The calculation is reduced to one-dimensional parametric integrals [see Eqs. (15) and (16)]. These expressions yield additional evidence for the results given in Eq. (17). We have not attempted to find analytic expressions for the remaining one- and two-dimensional integrations over the spectral parameter $\rho$ of the vacuum polarization, but note that such calculations may be possible [20, 21]; we leave this problem for future investigations.

The second point of the paper is the calculation of two nontrivial higher-order corrections to vacuum polarization in simple muonic bound systems: namely, the self-energy and recoil corrections to VP (see Secs. 3 and 4). For the self-energy correction to VP, the final numerical results are given in Eq. (29). Numerically, we confirm results reported previously in Ref. [13] for $\mu$H. The same analytic techniques are used as those employed in Sec. 2 but intermediate results are suppressed. In Eq. (23a), we take the opportunity to correct [13] a computational error in the evaluation of the self-energy correction for the matrix element $M_{60}$ which describes the vacuum-polarization correction to the electron anomalous magnetic moment term in the Lamb shift (the correction has negligible effect on

the numerical value of the final result). Our results include the correction to the Bethe logarithm due to vacuum polarization [see Eq. (25) and (26)].

The radiative-recoil correction is found to be numerically small for simple muonic bound systems. Leading and subleading logarithmic terms are calculated here. The first logarithmic term in the radiative-recoil correction is due to the vacuum-polarization correction to the frequency-dependent Breit exchange and is given in Eq. (35) [see Figs. 4(a) and (b)]. From the seagull part, the leading logarithm is given (for $S$ states) by the vacuum-polarization insertion into the exchange photon lines [see Figs. 4(c), (e), (f)]. The corresponding double-logarithmic term $\delta E_S$ can be expressed analytically, scales as $n^{-3}$ where $n$ is the principal quantum number, and can be found in Eq. (38). The appearance of the parameter $\beta_N$ in the result implies that the logarithmic coefficient depends on the mass ratio of muon and electron, as it should. Finally, the wave function correction to $S$ states which is nonvanishing, generates a third logarithm, $\delta E_W$, given in Eq. (43) [see also Fig. 4(d)]. The total results for the radiative-recoil correction (logarithmic terms) for the systems under investigation can be found in Eq. (46).

Self-energy corrections to vacuum polarization and radiative-recoil corrections are found to be of minor significance, in accordance with simple order-of-magnitude estimates. Still, the calculations are necessary in order to exclude a conceivable large logarithmic term in the higher-order effects as an explanation for (part of) the observed spectroscopic discrepancy [6]. Also, the calculation of the subleading logarithmic terms in the radiative-recoil correction clarifies the size of one of the traditionally most elusive corrections for two-body bound systems, in the case of a bound muon. Experiments on these systems are ongoing at PSI (Paul–Scherrer–Institute, Villigen).

## Acknowledgments

## A Breit Hamiltonian

The Breit Hamiltonian describes the fine- and hyperfine splitting in two-body systems in the order $(Z\alpha)^4$, exact to all orders in the mass ratio. For the $2P$–$2S$ Lamb shift, the relevant terms in the Breit Hamiltonian read

$$\delta H = \sum_{j=1}^{4} \delta H_j, \qquad \delta H_1 = -\frac{\boldsymbol{p}^4}{8m_\mu^3} - \frac{\boldsymbol{p}^4}{8m_N^3},$$

$$\delta H_2 = \left(\frac{1}{m_\mu^2} + \frac{\delta_I}{m_N^2}\right)\frac{\pi Z\alpha\,\delta^3(r)}{2},$$

$$\delta H_3 = -\frac{Z\alpha}{2m_\mu m_N}p^i\left(\frac{1}{r} + \frac{r^i r^j}{r^3}\right)p^j,$$

$$\delta H_4 = \frac{Z\alpha}{r^3}\left(\frac{1}{4m_\mu^2} + \frac{1}{2m_\mu m_N}\right)\boldsymbol{\sigma}\cdot\boldsymbol{L}, \qquad (47)$$

where the summation convention is used. Here, $\delta_I = 1$ for half-integer and $\delta_I = 0$ for integer nuclear spin (see [22]). The expectation values of of the Breit Hamiltonian, evaluated for the $2P_{1/2}$–$2S_{1/2}$ difference read as

$$L(2P_{1/2}-2S_{1/2}) = \begin{cases} \dfrac{(Z\alpha)^4\mu^3}{48\,m_N^2} & \delta_I = 1, \\[2mm] \dfrac{(Z\alpha)^4\mu^3}{12\,m_N^2} & \delta_I = 0, \end{cases} \qquad (48)$$

where we recall that $2P_{1/2}$ is energetically higher. The shift evaluates to

$$L(\mu\mathrm{H}) = 0.05747\,\mathrm{meV}, \qquad (49a)$$

$$L(\mu\mathrm{D}) = 0.06722\,\mathrm{meV}, \qquad (49b)$$

$$L(\mu\,{}^3\mathrm{He}^+) = 0.12654\,\mathrm{meV}, \qquad (49c)$$

$$L(\mu\,{}^4\mathrm{He}^+) = 0.29518\,\mathrm{meV}. \qquad (49d)$$

These results confirm entries in Ref. [10].

## B Reduced Green Functions

We use the reduced Green function $G'$ of the $2S$ state for general radial arguments,

$$G'_{2S}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \left\langle \boldsymbol{r}_1 \left| \left(\frac{1}{H_0 - E_{2S}}\right)' \right| \boldsymbol{r}_2 \right\rangle$$
$$= R_{2S}(r_1, r_2)\,Y_{00}(\hat{r}_1)\,Y_{00}^*(\hat{r}_2), \qquad (50)$$

where $R_{2S}(r_1, r_2)$ has the following representation,

$$R_{2S}(r_1, r_2) = -\frac{\alpha\,\mu^2\,\exp\left(-\frac{1}{2}\,(R_< + R_>)\right)}{4\,R_<\,R_>}$$

$$\times \left[4\,\mathrm{e}^{R_<}\,R_<\,(R_> - 2)\,R_> + Q(R_<, R_>)\right.$$

$$\left. -4\,R_<\,(R_< - 2)\,R_>(R_> - 2)\,F(R_<, R_>)\right]. \qquad (51)$$

Here, $R_< = \alpha\mu r_<$ and $R_> = \alpha\mu r_>$, with $r_< = \min(r_1, r_2)$, and $r_> = \max(r_1, r_2)$. The result (51) constitutes a confirmation of Eq. (23) of Ref. [11]. The function $F$ is expressed as

$$F(R_<, R_>) = \mathrm{Ei}(R_<) - 2\gamma_E - \ln(R_<\,R_>). \qquad (52a)$$

The exponential integral can be written as

$$\mathrm{Ei}(x) = \int_0^x \mathrm{d}t\, \frac{\mathrm{e}^t - 1}{t} + \gamma_E + \ln(|x|)$$

$$= -(\mathrm{P.V.}) \int_{-x}^\infty \mathrm{d}t\, \frac{\mathrm{e}^{-t}}{t} = -\mathrm{E}_1(-x)\,, \qquad (52\mathrm{b})$$

for real $x$ (positive or negative), where $\gamma_E = 0.577216\ldots$ is the Euler–Mascheroni constant. We denote the principal value by the symbol "P.V.". The polynomial $Q$ in Eq. (51) reads

$$Q(R_<, R_>) = -8\,(R_< + R_>) + 26\,R_<\,R_>\,(R_< + R_>)$$
$$+ R_<^2\,R_>^2\,(R_< + R_>) + 4\,(R_<^2 - 3R_<R_> + R_>^2)$$
$$- R_<\,R_>\,(2R_<^2 + 23R_<R_> + 2R_>^2)\,. \qquad (53)$$

Using the integrals listed in Appendix A, it is actually possible to calculate the wave function correction

$$\delta\phi_{nS} = \left(\frac{1}{E_{nS} - H_0}\right)' v_{\mathrm{vp}}|\phi_{nS}\rangle \qquad (54)$$

analytically, where $v_{\mathrm{vp}}$ is given in Eq. (5).

## C Integrals

In order to carry out the radial integrations in the calculation of the wave function perturbation

$$|\delta\psi_{n\ell_j}\rangle = \left(\frac{1}{E_0 - H_0}\right)' v_{\mathrm{vp}}|n\ell_j\rangle \qquad (55)$$

for $2S$ and $2P$, one needs integrals with integration domains $r \in (0, s)$, and $r \in (s, \infty)$, due to radial ordering. We give the results for two useful integrals of the first category:

$$\int_0^s \mathrm{d}r\, \mathrm{e}^{-a\,r}\, \ln(r) \qquad (56\mathrm{a})$$

$$= \frac{1}{a}\left[\mathrm{Ei}(-a\,s) - \gamma_E - \ln(a)\,\left(\mathrm{e}^{-a\,s} + 1\right)\right]\,,$$

$$\int_0^s \mathrm{d}r\, \mathrm{e}^{-a\,r}\, \mathrm{Ei}(b\,r) \qquad (56\mathrm{b})$$

$$= -\frac{1}{a}\left[\mathrm{Ei}\left((b-a)\,s\right) - \mathrm{e}^{-a\,s}\,\mathrm{Ei}\left(b\,s\right) + \ln\left(\left|\frac{b}{a-b}\right|\right)\right]$$

In the second category, the following expressions are relevant:

$$\int_s^\infty \mathrm{d}r\, \mathrm{e}^{-a\,r}\, \ln(r) = \frac{1}{a}\left[\mathrm{Ei}(-a\,s)\,\ln(a) - \mathrm{Ei}(-a\,s)\right]\,,$$
$$\qquad (57\mathrm{a})$$

$$\int_s^\infty \mathrm{d}r\, \mathrm{e}^{-a\,r}\, \mathrm{Ei}(b\,r) = \frac{1}{a}\left[\mathrm{Ei}\left((b-a)\,s\right) - \mathrm{e}^{-a\,s}\,\mathrm{Ei}\left(b\,s\right)\right]\,,$$
$$\qquad (57\mathrm{b})$$

where we note that the results are much more compact than for the first category. Finally, integrals over the interval $r \in (0, \infty)$ are needed for the evaluation of second-order matrix elements [see Eq. (9)]. One example is

$$\int_0^\infty \mathrm{d}r\, \mathrm{e}^{-a\,r}\, \mathrm{Ei}(b\,r)\, \ln(r) = \frac{\pi^2}{3\,a} + \frac{1}{2\,a}\,\ln^2\left[a(a-b)\right]$$

$$+ \frac{1}{a}\,\ln(a-b)\,\left[\gamma_E + \ln\left(\frac{a}{b}\right)\right]$$

$$- \frac{1}{a}\left[\gamma_E\,\ln(b) + \mathrm{Li}_2\left(\frac{a-b}{a}\right)\right]\,. \qquad (58)$$

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